

Reprocessing White Pagoda

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Code version: updated May 31, 2019

MANUALLY UPDATE: user defined, session-specific information

```
User <- "Marina"
session <- "DH2" #change this to whatever name or number you want to give you session, is appended on to plot titles and spreadsheet output so that everything is session specific, including file names
MS.ID<-"Bert" #don't change this unless we get a new mass spec or you are using this for data from another lab
:)
```

Install custom packages

These will change frequently over the next couple of years, so it is wise to reinstall them everytime, to be sure you are using the up-to-date versions of the functions that the code below needs. If there haven't been any changes to the codes, it will say that and not reinstall them.

```
devtools::install_github("KopfLab/isoreader")

devtools::install_github("cubessil/isoprocessCUBES") #general CUBESsil lab stuff

devtools::install_github("cubessil/CUBESSILclumpedmath") #only for processing clumped data
```

Load libraries and clumped isotope standard values

```
library(rlang)
library(plotly)
library(isoreader)
library(tidyverse)
library(isoprocessCUBES)
library(CUBESSILclumpedmath)
```

```
Standards <- readRDS(url("https://github.com/cubessil/clumpsRcodes/blob/master/Standards.RDS?raw=true"))
#ProjectIDs <- read.csv("ProjectIDs.csv") IMPLEMENT ~ lets start a data file of sample IDs and Project IDs, so we can leave this out of the functions, but have a good cross platform, can store as RDS and read it in from github as well....
```

Load all did files in a folder (or multiple folders)

Catches any errors and exceptions that might occur and reports them as "problems".

```
readrawdata <- TRUE
if (readrawdata){
  folder <- file.path(".",")
  stopifnot(file.exists(folder))
  tictoc::tic()
  did_files <- iso_read_dual_inlet(folder,cache = TRUE, quiet = FALSE, read_vendor_data_table = TRUE, parallel = TRUE)
  tictoc::toc()
  did_files <- iso_filter_files_with_problems(did_files)
  saveRDS(did_files, paste0(session, "_did_files.RDS"))
}else{
  did_files <- readRDS(paste0(session, "_did_files.RDS"))
}
```

```
## Info: preparing to read 3124 data files (all will be cached), setting up 16...
```

```
## Info (process 1): reading file './rawdata/190528/29823_all$zero_0.did' fro...
```

```
## Info (process 1): running compatibility checks for outdated cached file cre...
```

```
## Info (process 1): reading file './rawdata/190528/29839_ArtiersAriter_12_6_...
```

```
## Info (process 1): running compatibility checks for outdated cached file cre...
```

```
## Info (process 2): reading file './rawdata/190528/29824_all$zero_0.did' fro...
```

```
## Info (process 3): reading file './rawdata/190528/29825_all$zero_0.did' fro...
```

```
## Info (process 1): reading file './rawdata/190528/29855_ArtiersAriter_8_4_3...
```

```
## Info (process 2): running compatibility checks for outdated cached file cre...
```

```
## Info (process 1): running compatibility checks for outdated cached file cre...
```

```
## Info (process 3): running compatibility checks for outdated cached file cre...
```

```
## Info (process 4): reading file './rawdata/190528/29826_all$zero_0.did' fro...
```

```
## Info (process 2): reading file './rawdata/190528/29840_ArtiersAriter_12_6_...
```

```
## Info (process 1): reading file './rawdata/190528/29871_ArtiersAriter_7_5_5...
```

```
## Info (process 2): running compatibility checks for outdated cached file cre...
```

```
## Info (process 1): running compatibility checks for outdated cached file cre...
```

```
## Info (process 3): reading file './rawdata/190528/29841_ArtiersAriter_12_6_...
```

```
## Info (process 4): running compatibility checks for outdated cached file cre...
```

```
## Info (process 5): reading file './rawdata/190528/29827_all$zero_0.did' fro...
```

```
## Info (process 3): running compatibility checks for outdated cached file cre...
```

```
## Info (process 1): reading file './rawdata/190528/29887_ArtiersAriter_6_4_4...
```

```
## Info (process 2): reading file './rawdata/190528/29856_ArtiersAriter_8_4_3...
```

```
## Info (process 1): running compatibility checks for outdated cached file cre...
```

```
## Info (process 2): running compatibility checks for outdated cached file cre...
```

```
## Info (process 5): running compatibility checks for outdated cached file cre...
```

```
## Info (process 4): reading file './rawdata/190528/29842_ArtiersAriter_12_6_...
```

```
## Info (process 3): reading file './rawdata/190528/29857_ArtiersAriter_8_4_3...
```

```
## Info (process 6): reading file './rawdata/190528/29828_all$zero_0.did' fro...
```

```
## Info (process 4): running compatibility checks for outdated cached file cre...
```

```
## Info (process 10): reading file './rawdata/190716_ACF/32816__ACF$AF-NCF-TS-17-ElyL5_5_545.did' from cache...

## Info (process 4): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 13): reading file './rawdata/190715_ACF/32803__ACF$AF-NCF-TS2-16-28_5_880.did' from cache...

## Info (process 16): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 3): reading file './rawdata/190717_ACF/32937__all$ETH3_4_558.did' from cache...

## Info (process 9): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 6): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 8): reading file './rawdata/190716_ACF/32862__all$ETH2_7_725.did' from cache...

## Info (process 11): reading file './rawdata/190715_ACF/32801__ACF$AF-NCF-TS2-16-28_5_880.did' from cache...

## Info (process 12): reading file './rawdata/190715_ACF/32802__ACF$AF-NCF-TS2-16-28_5_880.did' from cache...

## Info (process 15): reading file './rawdata/190715_ACF/32773__ACF$AF-NCF-TS-17-ElyL5spar_4_141.did' from cache...

## Info (process 10): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 8): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 1): reading file './rawdata/190717_ACF/32903__all$IAEA-C2_4_132.did' from cache...

## Info (process 2): reading file './rawdata/190717_ACF/32920__ACF$AF-NCF-TS2-16-19_4_306.did' from cache...

## Info (process 3): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 7): reading file './rawdata/190716_ACF/32877__ACF$AF-NCF-TS2-16-28_6_102.did' from cache...

## Info (process 13): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 11): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 15): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 12): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 14): reading file './rawdata/190715_ACF/32804__ACF$AF-NCF-TS2-16-28_5_880.did' from cache...

## Info (process 5): reading file './rawdata/190717_ACF/32923__ACF$AF-NCF-TS2-16-19_4_306.did' from cache...

## Info (process 1): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 4): reading file './rawdata/190717_ACF/32938__all$ETH3_4_558.did' from cache...

## Info (process 2): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 16): reading file './rawdata/190715_ACF/32790__all$ETH1_5_896.did' from cache...

## Info (process 7): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 6): reading file './rawdata/190717_ACF/32940__all$ETH3_4_558.did' from cache...

## Info (process 5): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 10): reading file './rawdata/190716_ACF/32832__all$SSB-1000_0.did' from cache...

## Info (process 14): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 9): reading file './rawdata/190717_ACF/32879__ACF$AF-NCF-TS2-16-28_6_102.did' from cache...

## Info (process 16): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 4): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 6): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 13): reading file './rawdata/190716_ACF/32819__ACF$AF-NCF-TS2-17-21_5Bspar-gen2_5_630.did' from cache...

## Info (process 15): reading file './rawdata/190715_ACF/32789__ACF$AF-NCF-TS2-16-10_4_642.did' from cache...

## Info (process 10): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 3): reading file './rawdata/190717_ACF/32953__all$NBS19_4_449.did' from cache...

## Info (process 11): reading file './rawdata/190716_ACF/32817__ACF$AF-NCF-TS2-17-21_5Bspar-gen2_5_630.did' from cache...

## Info (process 9): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 12): reading file './rawdata/190716_ACF/32818__ACF$AF-NCF-TS2-17-21_5Bspar-gen2_5_630.did' from cache...

## Info (process 8): reading file './rawdata/190716_ACF/32878__ACF$AF-NCF-TS2-16-28_6_102.did' from cache...

## Info (process 7): reading file './rawdata/190717_ACF/32893__ACF$AF-NCF-TS2-16-19_5_252.did' from cache...

## Info (process 15): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 11): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 13): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 2): reading file './rawdata/190717_ACF/32936__all$ETH3_4_558.did' from cache...

## Info (process 3): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 8): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 1): reading file './rawdata/190717_ACF/32919__ACF$AF-NCF-TS2-16-19_4_306.did' from cache...
```



```
## Info (process 5): reading file './rawdata/190717_ACF/32939__all$ETH3_4_558.did' from cache...

## Info (process 12): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 7): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 14): reading file './rawdata/190716_ACF/32820__ACF$AF-NCF-TS2-17-21_5Bspar-gen2_5_630.did' from
cache...

## Info (process 2): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 4): reading file './rawdata/190717_ACF/32954__all$NBS19_4_449.did' from cache...

## Info (process 16): reading file './rawdata/190715_ACF/32806__ACF$AF-NCF-TS2-16-28_5_880.did' from cache...

## Info (process 1): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 6): reading file './rawdata/190717_ACF/32956__all$NBS19_4_449.did' from cache...

## Info (process 9): reading file './rawdata/190717_ACF/32895__ACF$AF-NCF-TS2-16-19_5_252.did' from cache...

## Info (process 5): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 14): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 4): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 16): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 10): reading file './rawdata/190716_ACF/32848__ACF$AF-NCF-TS-17-ElyLsSpar_6_371.did' from cach
e...

## Info (process 13): reading file './rawdata/190716_ACF/32835__all$IIEA-C1_6_795.did' from cache...

## Info (process 9): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 15): reading file './rawdata/190715_ACF/32805__ACF$AF-NCF-TS2-16-28_5_880.did' from cache...

## Info (process 6): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 3): reading file './rawdata/190717_ACF/32969__ACF$AF-NCF-TS2-17-21_5Bspar-gen2_2_769.did' from c
ache...

## Info (process 11): reading file './rawdata/190716_ACF/32833__all$SSB_1000_0.did' from cache...

## Info (process 8): reading file './rawdata/190717_ACF/32894__ACF$AF-NCF-TS2-16-19_5_252.did' from cache...

## Info (process 12): reading file './rawdata/190716_ACF/32834__all$SSB_1000_0.did' from cache...

## Info (process 7): reading file './rawdata/190717_ACF/32909__all$SSB_25_0.did' from cache...

## Info (process 10): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 11): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 3): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 13): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 2): reading file './rawdata/190717_ACF/32952__all$NBS19_4_449.did' from cache...

## Info (process 8): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 1): reading file './rawdata/190717_ACF/32935__all$ETH3_4_558.did' from cache...

## Info (process 12): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 15): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 14): reading file './rawdata/190716_ACF/32836__all$IIEA-C1_6_795.did' from cache...

## Info (process 5): reading file './rawdata/190717_ACF/32955__all$NBS19_4_449.did' from cache...

## Info (process 4): reading file './rawdata/190718_ACF/32970__all$zero_0.did' from cache...

## Info (process 7): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 2): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 16): reading file './rawdata/190716_ACF/32822__ACF$AF-NCF-TS2-17-21_5Bspar-gen2_5_630.did' from
cache...

## Info (process 1): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 14): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 5): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 9): reading file './rawdata/190717_ACF/32911__all$SSB_25_0.did' from cache...

## Info (process 4): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 10): reading file './rawdata/190716_ACF/32864__all$ETH2_7_725.did' from cache...

## Info (process 16): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 9): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 8): reading file './rawdata/190717_ACF/32910__all$SSB_25_0.did' from cache...

## Info (process 15): reading file './rawdata/190716_ACF/32821__ACF$AF-NCF-TS2-17-21_5Bspar-gen2_5_630.did' from
cache...

## Info (process 13): reading file './rawdata/190716_ACF/32851__ACF$AF-NCF-TS-17-ElyLsSpar_6_371.did' from cach
e...

## Info (process 7): reading file './rawdata/190717_ACF/32925__ACF$AF-NCF-TS2-16-28_6_063.did' from cache...
```

```
## Info (process 12): reading file './rawdata/190716_ACF/32850__ACF$AF-NCF-TS-17-ElyL5spar_6_371.did' from cach
e...

## Info (process 11): reading file './rawdata/190716_ACF/32849__ACF$AF-NCF-TS-17-ElyL5spar_6_371.did' from cach
e...

## Info (process 10): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 2): reading file './rawdata/190717_ACF/32968__ACF$AF-NCF-TS2-17-21_5Bspar-gen2_2_769.did' from c
ache...

## Info (process 13): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 8): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 1): reading file './rawdata/190717_ACF/32951__ACF$AF-NCF-TS2-16-10_8_790.did' from cache...

## Info (process 15): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 12): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 11): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 7): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 14): reading file './rawdata/190716_ACF/32852__ACF$AF-NCF-TS-17-ElyL5spar_6_371.did' from cach
e...

## Info (process 2): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 16): reading file './rawdata/190716_ACF/32838__all$IAEA-C1_6_795.did' from cache...

## Info (process 1): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 14): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 9): reading file './rawdata/190717_ACF/32927__ACF$AF-NCF-TS2-16-28_6_063.did' from cache...

## Info (process 16): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 10): reading file './rawdata/190717_ACF/32880__ACF$AF-NCF-TS2-16-10_5_932.did' from cache...

## Info (process 9): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 13): reading file './rawdata/190716_ACF/32867__all$ETH2_7_725.did' from cache...

## Info (process 15): reading file './rawdata/190716_ACF/32837__all$IAEA-C1_6_795.did' from cache...

## Info (process 12): reading file './rawdata/190716_ACF/32866__all$ETH2_7_725.did' from cache...

## Info (process 11): reading file './rawdata/190716_ACF/32865__all$ETH2_7_725.did' from cache...

## Info (process 8): reading file './rawdata/190717_ACF/32926__ACF$AF-NCF-TS2-16-28_6_063.did' from cache...

## Info (process 10): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 15): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 1): reading file './rawdata/190717_ACF/32967__ACF$AF-NCF-TS2-17-21_5Bspar-gen2_2_769.did' from c
ache...

## Info (process 12): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 13): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 7): reading file './rawdata/190717_ACF/32941__all$ETH3_4_558.did' from cache...

## Info (process 8): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 11): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 14): reading file './rawdata/190716_ACF/32868__all$ETH2_7_725.did' from cache...

## Info (process 1): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 7): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 16): reading file './rawdata/190716_ACF/32854__ACF$AF-NCF-TS2-16-10_4_226.did' from cache...

## Info (process 14): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 9): reading file './rawdata/190717_ACF/32943__ACF$AF-NCF-TS2-16-10_8_790.did' from cache...

## Info (process 10): reading file './rawdata/190717_ACF/32896__ACF$AF-NCF-TS2-16-19_5_252.did' from cache...

## Info (process 16): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 15): reading file './rawdata/190716_ACF/32853__ACF$AF-NCF-TS2-16-10_4_226.did' from cache...

## Info (process 8): reading file './rawdata/190717_ACF/32942__all$ETH3_4_558.did' from cache...

## Info (process 9): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 12): reading file './rawdata/190717_ACF/32882__ACF$AF-NCF-TS2-16-10_5_932.did' from cache...

## Info (process 13): reading file './rawdata/190717_ACF/32883__ACF$AF-NCF-TS2-16-10_5_932.did' from cache...

## Info (process 10): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 11): reading file './rawdata/190717_ACF/32881__ACF$AF-NCF-TS2-16-10_5_932.did' from cache...

## Info (process 7): reading file './rawdata/190717_ACF/32957__all$NBS19_4_449.did' from cache...

## Info (process 15): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 12): running compatibility checks for outdated cached file created by isoreader version < 1.2.0
```

```
## Info (process 13): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 8): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 11): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 7): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 14): reading file './rawdata/190717_ACF/32884__ACFSAF-NCF-TS2-16-10_5_932.did' from cache...

## Info (process 16): reading file './rawdata/190716_ACF/32870__all$ETH2_7_725.did' from cache...

## Info (process 9): reading file './rawdata/190717_ACF/32959__all$NBS19_4_449.did' from cache...

## Info (process 14): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 10): reading file './rawdata/190717_ACF/32912__all$eSSB_25_0.did' from cache...

## Info (process 16): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 15): reading file './rawdata/190716_ACF/32869__all$ETH2_7_725.did' from cache...

## Info (process 12): reading file './rawdata/190717_ACF/32898__all$IAEA-C2_4_132.did' from cache...

## Info (process 9): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 8): reading file './rawdata/190717_ACF/32958__all$NBS19_4_449.did' from cache...

## Info (process 13): reading file './rawdata/190717_ACF/32899__all$IAEA-C2_4_132.did' from cache...

## Info (process 11): reading file './rawdata/190717_ACF/32897__ACFSAF-NCF-TS2-16-19_5_252.did' from cache...

## Info (process 15): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 10): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 12): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 8): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 13): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 11): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 14): reading file './rawdata/190717_ACF/32980__all$IAEA-C2_4_132.did' from cache...

## Info (process 16): reading file './rawdata/190717_ACF/32886__ACFSAF-NCF-TS2-16-10_5_932.did' from cache...

## Info (process 14): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 10): reading file './rawdata/190717_ACF/32928__ACFSAF-NCF-TS2-16-28_6_063.did' from cache...

## Info (process 16): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 12): reading file './rawdata/190717_ACF/32914__all$eSSB_25_0.did' from cache...

## Info (process 15): reading file './rawdata/190717_ACF/32885__ACFSAF-NCF-TS2-16-10_5_932.did' from cache...

## Info (process 13): reading file './rawdata/190717_ACF/32915__all$eSSB_25_0.did' from cache...

## Info (process 10): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 12): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 15): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 11): reading file './rawdata/190717_ACF/32913__all$eSSB_25_0.did' from cache...

## Info (process 13): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 14): reading file './rawdata/190717_ACF/32916__ACFSAF-NCF-TS2-16-19_4_386.did' from cache...

## Info (process 11): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 16): reading file './rawdata/190717_ACF/32902__all$IAEA-C2_4_132.did' from cache...

## Info (process 14): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 10): reading file './rawdata/190717_ACF/32944__ACFSAF-NCF-TS2-16-10_8_798.did' from cache...

## Info (process 12): reading file './rawdata/190717_ACF/32930__ACFSAF-NCF-TS2-16-28_6_063.did' from cache...

## Info (process 15): reading file './rawdata/190717_ACF/32901__all$IAEA-C2_4_132.did' from cache...

## Info (process 16): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 12): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 10): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 13): reading file './rawdata/190717_ACF/32931__ACFSAF-NCF-TS2-16-28_6_063.did' from cache...

## Info (process 15): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 11): reading file './rawdata/190717_ACF/32929__ACFSAF-NCF-TS2-16-28_6_063.did' from cache...

## Info (process 14): reading file './rawdata/190717_ACF/32932__ACFSAF-NCF-TS2-16-28_6_063.did' from cache...

## Info (process 13): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 11): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 16): reading file './rawdata/190717_ACF/32918__ACFSAF-NCF-TS2-16-19_4_386.did' from cache...

## Info (process 14): running compatibility checks for outdated cached file created by isoreader version < 1.2.0
```

```
## Info (process 12): reading file './rawdata/190717_ACF/32946__ACFSAF-NCF-TS2-16-10_8_790.did' from cache...

## Info (process 15): reading file './rawdata/190717_ACF/32917__ACFSAF-NCF-TS2-16-19_4_306.did' from cache...

## Info (process 10): reading file './rawdata/190717_ACF/32960__all$NBS19_4_449.did' from cache...

## Info (process 16): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 13): reading file './rawdata/190717_ACF/32947__ACFSAF-NCF-TS2-16-10_8_790.did' from cache...

## Info (process 10): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 12): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 15): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 11): reading file './rawdata/190717_ACF/32945__ACFSAF-NCF-TS2-16-10_8_790.did' from cache...

## Info (process 14): reading file './rawdata/190717_ACF/32948__ACFSAF-NCF-TS2-16-10_8_790.did' from cache...

## Info (process 13): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 11): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 16): reading file './rawdata/190717_ACF/32934__all$ETH3_4_558.did' from cache...

## Info (process 14): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 15): reading file './rawdata/190717_ACF/32933__ACFSAF-NCF-TS2-16-28_6_063.did' from cache...

## Info (process 12): reading file './rawdata/190717_ACF/32962__ACFSAF-NCF-TS2-17-21_5Bspar-gen2_2_769.did' from cache...

## Info (process 16): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 12): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 15): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 13): reading file './rawdata/190717_ACF/32963__ACFSAF-NCF-TS2-17-21_5Bspar-gen2_2_769.did' from cache...

## Info (process 11): reading file './rawdata/190717_ACF/32961__ACFSAF-NCF-TS2-17-21_5Bspar-gen2_2_769.did' from cache...

## Info (process 14): reading file './rawdata/190717_ACF/32964__ACFSAF-NCF-TS2-17-21_5Bspar-gen2_2_769.did' from cache...

## Info (process 13): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 16): reading file './rawdata/190717_ACF/32950__ACFSAF-NCF-TS2-16-10_8_790.did' from cache...

## Info (process 11): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 14): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 15): reading file './rawdata/190717_ACF/32949__ACFSAF-NCF-TS2-16-10_8_790.did' from cache...

## Info (process 16): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 15): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 16): reading file './rawdata/190717_ACF/32966__ACFSAF-NCF-TS2-17-21_5Bspar-gen2_2_769.did' from cache...

## Info (process 15): reading file './rawdata/190717_ACF/32965__ACFSAF-NCF-TS2-17-21_5Bspar-gen2_2_769.did' from cache...

## Info (process 16): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info (process 15): running compatibility checks for outdated cached file created by isoreader version < 1.2.0

## Info: finished reading 3124 files in 34.24 secs

## Warning: some files were read from outdated cache or storage (.rds) files. They
## were checked for compatibility and should work without issues. However, to avoid
## this warning and improve read speed, please call iso_reread_outdated_files() on
## your collection of iso files to refresh outdated cache files.

## Info: encountered 3408 problems in total

## # A tibble: 3,408 x 4
##   file_id      type    func    details
##   <chr>      <chr>    <chr>    <chr>
## 1 29823_all$zero_0.did warnl_ read_iso_ cache file created by an outdated v_
## 2 29839_Artier$Arter_1_ warnl_ read_iso_ cache file created by an outdated v_
## 3 29855_Artier$Arter_8_ warnl_ read_iso_ cache file created by an outdated v_
## 4 29871_Artier$Arter_7_ warnl_ read_iso_ cache file created by an outdated v_
## 5 29887_Artier$Arter_6_ warnl_ read_iso_ cache file created by an outdated v_
## 6 29903_all$CU_YULE_4_1_ warnl_ read_iso_ cache file created by an outdated v_
## 7 29928_all$ES58_25_0_ warnl_ read_iso_ cache file created by an outdated v_
## 8 29944_Layzell$Layzell_ warnl_ read_iso_ cache file created by an outdated v_
## 9 29960_Layzell$Layzell_ warnl_ read_iso_ cache file created by an outdated v_
## 10 29976_Layzell$Layzell_ warnl_ read_iso_ cache file created by an outdated v_
## # _ with 3,398 more rows
##
## # 36.997 sec elapsed

## Info: removing 97/3124 files that have any error (keeping 3027)

rawdata <- prep_didfiles(did_files)

## Info: aggregating standards info from 3027 data file(s)

## Info: aggregating raw data from 3027 data file(s), including file info 'c(Analysis, file_datetime, Preparatio
n, Identifier 1, Identifier 2, MS_integration_time.s, Method, measurement_info)'

#code example for fixing batching problems when making the flatlist.cyc dataframe:
#rawdata[ rawdata$Analysis > 30125 & rawdata$Analysis < 30125, "Preparation"] <- "D" #to fix two back to back
dr_1000 that didn't have different preparation labels and so didn't batch correctly

#clump math
```

```
flatlist.Cyc <- clumpedbyCyc(rawdata)
```

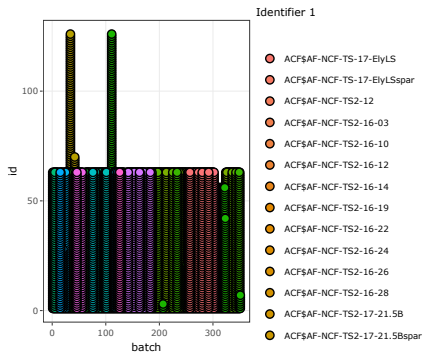
```
## Warning: All elements of `...` must be named.
## Did you want `data = c(Analysis, file_datetime, Preparation, `Identifier 1`, `Identifier 2`,
##   MS_integration_time.s, Method, measurement_info, type, cycle,
##   v44.mV, v45.mV, v46.mV, v47.mV, v48.mV, v49.mV, v54.mV, `ref d 13C/12C`,
##   `ref d 18O/16O`)?`
```

```
#flatlist.Cyc.017 <- clumpedbyCyc(rawdata, lambda = 0.528) #for illustration purposes only
```

```
#this plots batch versus id, and is colored by Identifier 1. This is a visual way to assess if all the samples we
re correctly batch. Watch samples with an abnormal number of cycles (ie, id number) and different colors, which s
uggests that samples didn't get binned correctly or there are 2 samples with the same name in a row that are bein
g counted as a single sample (e.g. running 2 of the same heated gas or standard in a row)
```

```
batching <- flatlist.Cyc %>%
  ggplot(aes(x=batch, y=id, fill = `Identifier 1`)) +
  geom_point(size = 3, shape = 21) +
  theme_bw()
```

```
ggplotly(batching)
```



```
unique(flatlist.Cyc$`Identifier 1`) #shows all unique sample ID names, so easy to see if there are inconsisten
cies that need to be fixed in the next box
```

```

## [1] "allzero"
## [2] "Artier$Arter_12"
## [3] "all$SB_1000"
## [4] "Artier$Arter_8"
## [5] "Artier$Arter_5"
## [6] "Artier$Arter_7"
## [7] "Artier$Arter_6"
## [8] "all$ETH2"
## [9] "all$CU_YULE"
## [10] "all$DR_25"
## [11] "all$SB_25"
## [12] "Layzell$Layzell-5.3-PLCT"
## [13] "Layzell$Layzell-5.3-MCL"
## [14] "Layzell$Layzell-10.1-MCL-1"
## [15] "Layzell$Layzell-10.1-MCL-2"
## [16] "all$ETH3"
## [17] "Layzell$Layzell-10.7-PLCT"
## [18] "all$IAEA-C1"
## [19] "Layzell$Layzell-10.4-PLCT-2"
## [20] "all$DR_1000"
## [21] "all$ETH1"
## [22] "Rehmus$Pin 218.24"
## [23] "Rehmus$Pin 137.85"
## [24] "Rehmus$Pin 278.36"
## [25] "Rehmus$Pin 185.34"
## [26] "Rehmus$Pin 223.56"
## [27] "all$IAEA-C2"
## [28] "Rehmus$Pin 178.36"
## [29] "all$SB_25"
## [30] "Artier$Arter_10"
## [31] "all$Merk"
## [32] "all$SB_1000"
## [33] "Layzell$Layzell_5.3_PLCT"
## [34] "Layzell$Layzell_5.3_MCL"
## [35] "Layzell$Layzell_1.1_MCL-1"
## [36] "Layzell$Layzell_1.1_MCL-2"
## [37] "Artier$Arter_13"
## [38] "Artier$Arter_9"
## [39] "Artier$Arter_11"
## [40] "Layzell$Layzell_10.4_PLCT-3"
## [41] "Layzell$Layzell_10.4_MCL-2"
## [42] "Layzell$Layzell-10.1 MCL-1"
## [43] "Layzell$Layzell-10.1 MCL-2"
## [44] "Layzell$Layzell-10.4 MCL-2"
## [45] "Layzell$Layzell-10.4 PLCT-3"
## [46] "Layzell$Layzell-10.4 MCL-4"
## [47] "Layzell$Layzell-10.7 MCL"
## [48] "Thomas$M9A_ISU"
## [49] "Thomas$M9A_ISU"
## [50] "Thomas$M43A_ISU"
## [51] "Thomas$M289A_ISU"
## [52] "Hanna$MTL-1532"
## [53] "Hanna$MTL-1536 N3-5P"
## [54] "Hanna$MTL-1509"
## [55] "Hanna$MTL-1536 N3"
## [56] "Meade$MB140527.ML.05.01.CN"
## [57] "Meade$MB140527.ML.float.CN.near.by.in.profl"
## [58] "Meade$MLUP-3.47cm.CN"
## [59] "Meade$MLUP-1.CN.base.of.pit"
## [60] "Meade$MB140527.CR.SPT.45cm.CN"
## [61] "Meade$MB140527.CR.SPT.85cm.CN"
## [62] "Meade$MB140527.CR.SPT.75cm.CN"
## [63] "Meade$MB140527.CR.SPT.60cm.CN"
## [64] "Meade$MB140607.RR3.100.002.CN"
## [65] "Meade$MB140527.RRT.SPT.50.03.CN"
## [66] "Meade$MLUP-3.20cm.CN"
## [67] "Meade$MB140527.RRT.SPT.40.02.CN"
## [68] "Meade$MB140527.CT2.SPT.65cm.CN"
## [69] "Meade$MB140527.CR.SPT.35cm.CN"
## [70] "Meade$MB140527.RRT.100cm.CN"
## [71] "all$ETH4"
## [72] "ACFSAF-NCF-TS2-16-03"
## [73] "ACFSAF-NCF-TS2-16-12"
## [74] "ACFSAF-NCF-TS2-16-14"
## [75] "ACFSAF-NCF-TS2-16-22"
## [76] "ACFSAF-NCF-TS-17-ELYLS"
## [77] "ACFSAF-NCF-TS-17-ELYLSspar"
## [78] "ACFSAF-NCF-TS2-17-21.5B"
## [79] "ACFSAF-NCF-TS2-17-21.5Bspar"
## [80] "ACFSAF-NCF-TS2-16-26"
## [81] "ACFSAF-NCF-TS2-16-24"
## [82] "all$NBS19"
## [83] "ACFSAF-NCF-TS2-22"
## [84] "ACFSAF-NCF-TS2-12"
## [85] "WP201153F-019"
## [86] "WP201153-021core"
## [87] "WP201156-042"
## [88] "WP201153H-014"
## [89] "WP201156-003"
## [90] "WP201153E-001"
## [91] "WP201154-03B"
## [92] "WP201153B-021"
## [93] "WP201153A-097"
## [94] "WP201153E-001clean"
## [95] "WP201153-0211cm"
## [96] "WP201156-003bwn"
## [97] "ACFSAF-NCF-TS2-17-21.5Bspar-gen2"
## [98] "ACFSAF-NCF-TS2-16-10"
## [99] "ACFSAF-NCF-TS2-16-28"
## [100] "ACFSAF-NCF-TS2-16-19"

```

#change names, add comments, and Donotuse

```

#Code examples:
#flatlist.Cyc[ flatlist.Cyc$Analysis > 28131 & flatlist.Cyc$Analysis < 28139.8, "Identifier 1"] <- "all5dR_1000"
#flatlist.Cyc[ flatlist.Cyc$Identifier 1 == "KB_CI_576; EBOC" , "Identifier 1"] <- "eBOC_1000"
#flatlist.Cyc <- getmetadatafromAnalysis(flatlist.Cyc, 28207, 28215.7, 28198) #Can use this function to shift the
metadata from one set of analysis numbers to another set; useful for occasions like carousel glitches or starting
the sequence on the wrong line that result in the wrong sample information for a given sample

#pulled from May and June, name fixes from katie -> May 2019
flatlist.Cyc[ flatlist.Cyc$Analysis > 29557 & flatlist.Cyc$Analysis < 29565.8, "Identifier 1"] <- "all5CU YULE"
flatlist.Cyc[ flatlist.Cyc$Analysis > 30223 & flatlist.Cyc$Analysis < 30231.8, "Identifier 1"] <- "RehmsSPin 17
8.36"
#flatlist.Cyc[ flatlist.Cyc$Analysis > 30449 & flatlist.Cyc$Analysis < 30457.8, "Identifier 1"] <- "all5eSSB_25"
flatlist.Cyc[ flatlist.Cyc$Analysis > 30356 & flatlist.Cyc$Analysis < 30361.8, "Identifier 1"] <- "all5dR_25"
flatlist.Cyc[ flatlist.Cyc$Analysis > 30765 & flatlist.Cyc$Analysis < 30773.8, "Identifier 1"] <- "all5eSSB_25"
flatlist.Cyc[ flatlist.Cyc$Analysis > 30449 & flatlist.Cyc$Analysis < 30457.8, "Identifier 1"] <- "all5eSSB_100
0"
flatlist.Cyc[ flatlist.Cyc$Identifier 1 == "all5Merk", "Identifier 1"] <- "all5Merck"

flatlist.Cyc[ flatlist.Cyc$Analysis > 31836 & flatlist.Cyc$Analysis < 31844.8, "Identifier 1"] <- "ACFSAF-NCF-TS
2-16-26" #sequence error where i forgot a normalrun_start caused the carousel to get behind by one compared to
the sequence labelling.so AF-NCF-TS2-16-26 was mislabeled as AF-NCF-TS2-16-24

flatlist.Cyc[ flatlist.Cyc$Analysis > 31980 & flatlist.Cyc$Analysis < 31988.8, "Identifier 1"] <- "ACFSAF-NCF-TS
2-16-22"
flatlist.Cyc[ flatlist.Cyc$Analysis > 31989 & flatlist.Cyc$Analysis < 31997.8, "Identifier 1"] <- "ACFSAF-NCF-TS
2-16-12"

flatlist.Cyc <- getmetadatafromAnalysis(flatlist.Cyc, 29988,29991.8,29979)
flatlist.Cyc <- getmetadatafromAnalysis(flatlist.Cyc, 29979,29987.8,29970)
flatlist.Cyc <- getmetadatafromAnalysis(flatlist.Cyc, 29970,29978.8,29961)
flatlist.Cyc <- getmetadatafromAnalysis(flatlist.Cyc, 29961,29969.8,29952)
flatlist.Cyc <- getmetadatafromAnalysis(flatlist.Cyc, 29952,29960.8,29943)
flatlist.Cyc <- getmetadatafromAnalysis(flatlist.Cyc, 29943,29951.8,29934)
flatlist.Cyc <- getmetadatafromAnalysis(flatlist.Cyc, 29934,29942.8,29929)
flatlist.Cyc <- getmetadatafromAnalysis(flatlist.Cyc, 29929,29933.8,29928)
flatlist.Cyc <- getmetadatafromAnalysis(flatlist.Cyc, 30356,30361.8,30357)#miss labeled

flatlist.Cyc <- getmetadatafromAnalysis(flatlist.Cyc, 30999,31007.8,30990)
flatlist.Cyc <- getmetadatafromAnalysis(flatlist.Cyc, 30990,30998.8,30981)
flatlist.Cyc <- getmetadatafromAnalysis(flatlist.Cyc, 30981,30989.8,30972)
flatlist.Cyc <- getmetadatafromAnalysis(flatlist.Cyc, 30972,30980.8,30963)

## filtering out all NOT "all" and "MP2011"
#
flatlist.Cyc <- flatlist.Cyc %>% filter(sub("\\$.*", "", sub("/$.*", "", 'Identifier 1'))=="all" | sub("\\$.
*", "", sub("/$.*", "", 'Identifier 1'))=="MP2011")
#flatlist.Cyc <- flatlist.Cyc %>% filter('Identifier 1' != "allzero" & Analysis > 31485 ) #get rid of oldzeros
#flatlist.Cyc <- flatlist.Cyc %>% filter(Analysis > 29038) #Anne's July run starts at Analysis31489 31052

#Add more outlier test

flatlist.Cyc <- flatlist.Cyc %>% ##prep dataframe, could be function but users should be able to make new outli
er col
group_by(batch) %>%
mutate(D47full.stdev = sd(D47full), D47full.mean =mean(D47full),
D47.outlier.1sig = abs(D47full.mean-D47full)>abs(D47full.stdev*1),
D47.outlier.2sig = abs(D47full.mean-D47full)>abs(D47full.stdev*2),
D47.outlier.3sig = abs(D47full.mean-D47full)>abs(D47full.stdev*3),
noutlier = FALSE)

#Yield Plots and signal Gas in these plots it to find samples or gases with too little gas that should not be used. 1st plot shows all cycles for all
acquisitions. Yield values after the first acquisition are equivalent to the percent bellows compression. If there is enough gas, "yield" should
increase after the first acquisition, and then should consistently drop after each acquisition. The lower plot shows just the first acquisition. The
second plot shows mass versus yield; samples that have <100% carbonate or have a yield issue (ie, not complete reaction) will fall off the main
line. Everything a zero is a reference gas. The last plot is mass 44 versus analysis. Samples that do not have enough sample to run will eventually
stop making it to 12.5 volts.

pYield.all <- flatlist.Cyc %>%
ggplot(aes(x=Analysis, y=Yield, fill = 'Preparation')) +
geom_point(shape = 21)

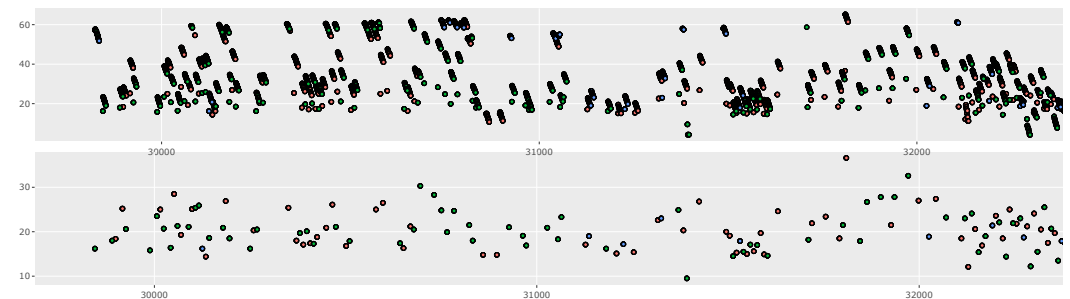
pYield.firstacq <- flatlist.Cyc %>%
filter(Method == "Start and Transfer.met") %>%
ggplot(aes(x=Analysis, y=Yield, fill = 'Preparation')) +
geom_point(shape = 21)

pYieldVmass <- flatlist.Cyc %>%
filter(Method == "Start and Transfer.met" & 'Identifier 2' != 0) %>%
ggplot(aes(x=as.numeric('Identifier 2'), y=Yield, fill = 'Preparation', label = 'Analysis')) +
geom_point(shape = 21)

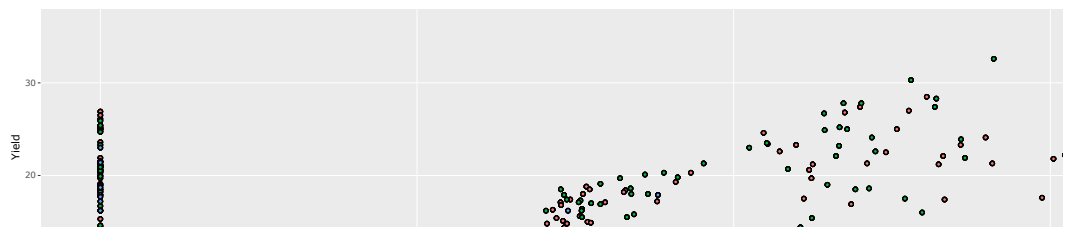
pM44mv <- flatlist.Cyc %>%
ggplot(aes(x=Analysis, y=v44.mV, fill='Preparation', label='Identifier 1')) +
geom_point(shape = 21)

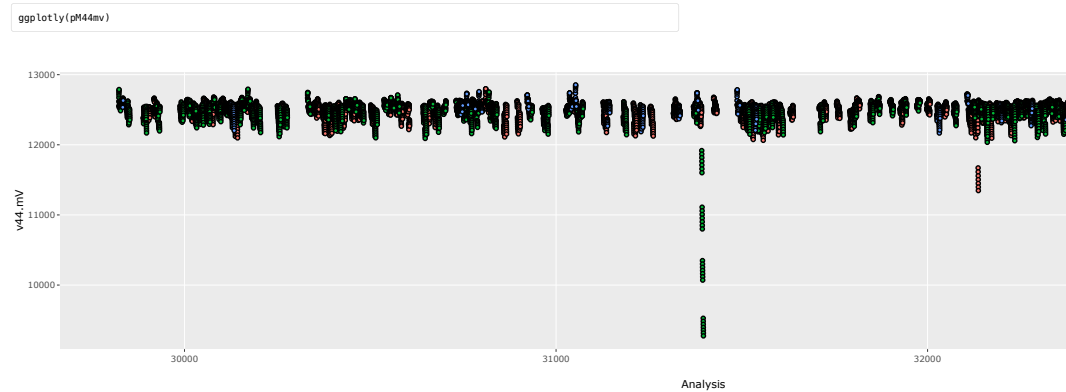
subplot(pYield.all, pYield.firstacq, nrow = 2)

```



```
ggplotly(pYieldVmass)
```





#add comments and Donotuse

```
#pulled from May and June, name fixes from katie -> May 2019
flatlist.Cyc[ flatlist.Cyc$Analysis > 29557 & flatlist.Cyc$Analysis < 29565.8, "Identifier 1"] <- "all$CUC YULE"
flatlist.Cyc[ flatlist.Cyc$Analysis > 30223 & flatlist.Cyc$Analysis < 30231.8, "Identifier 1"] <- "RehmuspIn 17
8.36"
#flatlist.Cyc[ flatlist.Cyc$Analysis > 30449 & flatlist.Cyc$Analysis < 30457.8, "Identifier 1"] <- "all$SSB_25"
flatlist.Cyc[ flatlist.Cyc$Analysis > 30356 & flatlist.Cyc$Analysis < 30361.8, "Identifier 1"] <- "all$dR_25"
flatlist.Cyc[ flatlist.Cyc$Analysis > 30765 & flatlist.Cyc$Analysis < 30773.8, "Identifier 1"] <- "all$SSB_25"
flatlist.Cyc[ flatlist.Cyc$Analysis > 30449 & flatlist.Cyc$Analysis < 30457.8, "Identifier 1"] <- "all$SSB_100
0"
flatlist.Cyc[ flatlist.Cyc$Identifier 1 == "all$Merk", "Identifier 1"] <- "all$Merck"

flatlist.Cyc[ flatlist.Cyc$Analysis > 31836 & flatlist.Cyc$Analysis < 31844.8, "Identifier 1"] <- "ACFSAF-NCF-TS
2-16-26" #sequence error where i forgot a normalrun_start caused the carousel to get behind by one compared to
the sequence labelling.so AF-NCF-TS2-16-26 was mislabeled as AF-NCF-TS2-16-24

flatlist.Cyc[ flatlist.Cyc$Analysis > 31980 & flatlist.Cyc$Analysis < 31988.8, "Identifier 1"] <- "ACFSAF-NCF-TS
2-16-22"
flatlist.Cyc[ flatlist.Cyc$Analysis > 31989 & flatlist.Cyc$Analysis < 31997.8, "Identifier 1"] <- "ACFSAF-NCF-TS
2-16-12"

flatlist.Cyc <- flatlist.Cyc %>%
  change.donotuse.and.runinfo(31392,31396,TRUE,"less then 12.5V") %>% #dR_1000
  change.donotuse.and.runinfo(31612,31621,FALSE,"stir stick maybe thrown. monitor against further replicates") %
>% #ACFSAF-NCF-TS2-16-03
  change.donotuse.and.runinfo(31621,31630,FALSE,"stir stick maybe thrown. monitor against further replicates") %
>% #ACFSAF-NCF-TS2-16-12
  change.donotuse.and.runinfo(31630,31638,FALSE,"stir stick maybe thrown. monitor against further replicates") %
>% #all$ETH1
  change.donotuse.and.runinfo(31639,31648,FALSE,"stir stick maybe thrown. monitor against further replicates") %
>% #ACFSAF-NCF-TS2-16-14
  change.donotuse.and.runinfo(31648,31657,FALSE,"stir stick maybe thrown. monitor against further replicates") %
>% #ACFSAF-NCF-TS2-16-22
  change.donotuse.and.runinfo(31708.1,31708.4,TRUE,"zero was cut short") %>% #zero was cut short
  change.donotuse.and.runinfo(31827.1,31836,TRUE,"not enough and sequence error, no gas dropped so this sample
just ran previous sample's gas") %>%
  change.donotuse.and.runinfo(31827.1,31836,TRUE,"low yield. less than 12.5V") %>%
  change.donotuse.and.runinfo(31908.1,31917,TRUE,"low yield. less than 12.5V") %>%
  change.donotuse.and.runinfo(29625.1,29633.7,TRUE,"offset from the rest of population of dR_25, keep eye on")%>%
  change.donotuse.and.runinfo(32136.1,32136.7,TRUE,"low yield")
#change.donotuse.and.runinfo(31917.1,31926,TRUE,"bulk isotopes differ greatly from other replicates")

#Example code:
# flatlist.Cyc <- flatlist.Cyc %>%
#   change.donotuse.and.runinfo(27150,27820,TRUE,"ong BRettt")

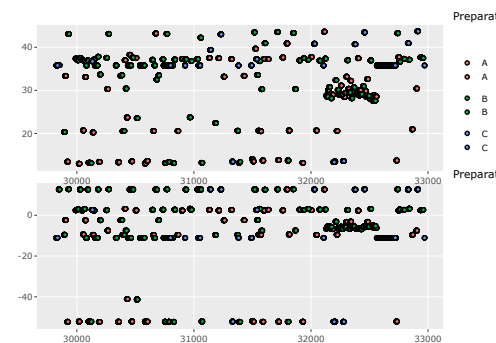
#note that when using Analysis numbers from the flatlist.Cyc dataframe, the analyses include .1 to .7 at the end
of each number. So, you need to account for that when defining the ranges. The function is set to read <= and >=
for the upper and lower bounds, respectively.
```

look at bulk isotopes - look for major fliers or samples with large variability

```
pd180 <- flatlist.Cyc %>%
  filter(Donotuse != TRUE) %>%
  ggplot(aes(x=Analysis, y=d180, fill='Preparation')) + geom_point()

pd13C <- flatlist.Cyc %>%
  filter(Donotuse != TRUE) %>%
  ggplot(aes(x=Analysis, y=d13C, fill='Preparation')) + geom_point()

subplot(pd180,pd13C,nrows = 2)
```



look at plots of all cycles for individual samples versus analysis number for d13C, d180, d13C V d180, and D47 versus analysis number. Looking for outlier cycles or acquisition, acquisitions with high variability relative to others in the sample, and other analytical problems (e.g. correlation between d13C and d180, strong trends in values at the cycle and/or acquisition level)


```
d180.mean <- flatlist.Cyc %>%
  filter(Donotuse != TRUE) %>%
  calc_means("d180", "batch", "Identifier 1")

p.ind.d180 <- flatlist.Cyc %>%
  filter(Donotuse != TRUE) %>%
  ggplot() +
  geom_hline(
    data = d180.mean,
    mapping = aes(yintercept = yintercept, linetype = linetype, color = id)) +
  geom_point(aes(x=Analysis, y=d180, fill = 'Identifier 1', shape = D47.outlier.2sig)) +
  scale_linetype_manual(values = c(1, 3, 2, 3, 2)) +
  scale_shape_manual(values = c(21, 24)) +
  facet_wrap(~batch, scales = "free") +
  theme_bw() +
  guides(linetype = "none")

d13C.mean <-
  flatlist.Cyc %>%
  filter(Donotuse != TRUE) %>%
  calc_means("d13C", "batch", "Identifier 1")

p.ind.d13C <- flatlist.Cyc %>%
  filter(Donotuse != TRUE) %>%
  ggplot() +
  geom_hline(
    data = d13C.mean,
    mapping = aes(yintercept = yintercept, linetype = linetype, color = id)) +
  geom_point(aes(x=Analysis, y=d13C, fill = 'Identifier 1', shape = D47.outlier.2sig)) +
  scale_linetype_manual(values = c(1, 3, 2, 3, 2)) +
  scale_shape_manual(values = c(21, 24)) +
  facet_wrap(~batch, scales = "free") +
  theme_bw() +
  guides(linetype = "none")

p.ind.d13Cvd180 <- flatlist.Cyc %>%
  filter(Donotuse != TRUE) %>%
  ggplot(aes(x=d180, y=d13C, fill='Identifier 1')) +
  geom_point(aes(shape = , shape = D47.outlier.2sig)) +
  scale_shape_manual(values = c(21, 24)) +
  facet_wrap(~batch, scales = "free") +
  theme_bw()

D47.mean <-
  flatlist.Cyc %>%
  filter(Donotuse != TRUE) %>%
  calc_means("D47full", "batch", "Identifier 1")

p.ind.D47 <- flatlist.Cyc %>%
  filter(Donotuse != TRUE) %>%
  ggplot() +
  geom_hline(
    data = D47.mean,
    mapping = aes(yintercept = yintercept, linetype = linetype, color = id)) +
  geom_point(aes(x=Analysis, y=D47full, fill = 'Identifier 1', shape = D47.outlier.2sig)) +
  scale_linetype_manual(values = c(1, 3, 2, 3, 2)) +
  scale_shape_manual(values = c(21, 24)) +
  facet_wrap(~batch, scales = "free") +
  theme_bw() +
  guides(linetype = "none")

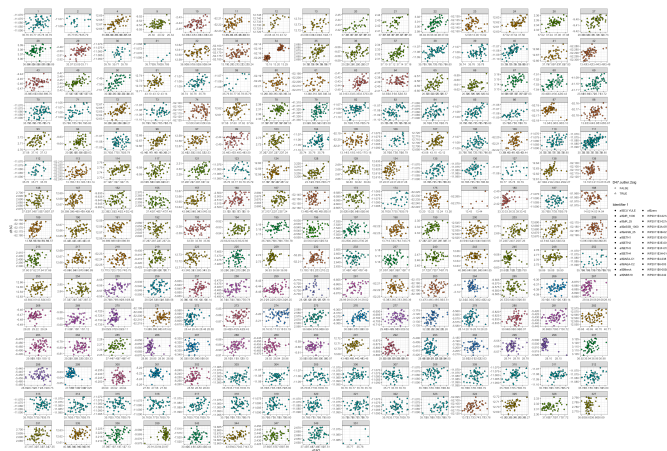
p.ind.d180
```



p.ind.d13C



p.ind.d13Cvd180



p.ind.D47



ID analysis number that correspond to problematic batch numbers, to make the donutuse labelling process easier

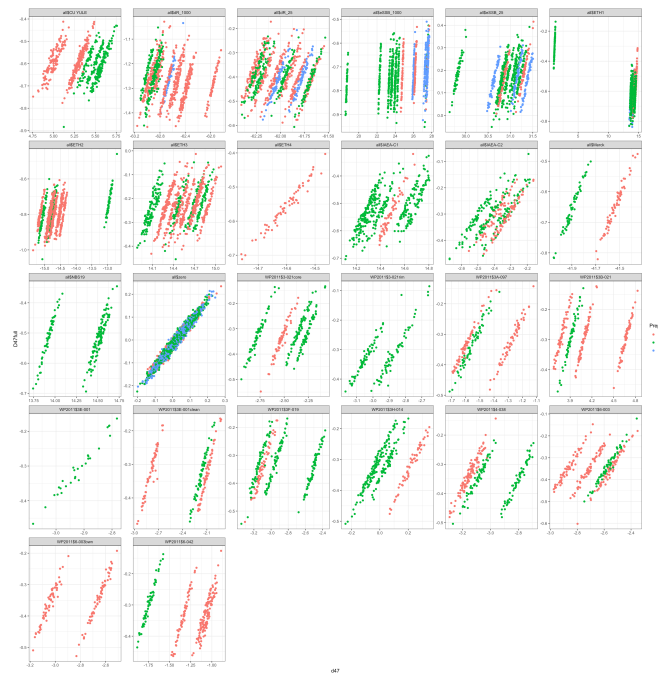
Plotting d180 and d13C by ID

```
flatlist.Cyc %>%
  filter(Donotuse != TRUE) %>%
  ggplot(aes(x=d180, y=d13C, color=Preparation, label = Analysis)) +
  geom_point() +
  facet_wrap(~ 'Identifier 1', scales = "free") +
  theme_bw()
```



Plotting D47 and d47 by ID

```
flatlist.Cyc %>%
  filter(Donotuse != TRUE) %>%
  ggplot(aes(x=d47, y=D47full, color=Preparation, label=Analysis)) +
  geom_point() +
  facet_wrap(~ 'Identifier 1', scales = "free") +
  theme_bw()
```



#add more comments and Donutuse, based on analytical issues and major outliers

```
#Example code:
# flatlist.Cyc <- flatlist.Cyc %>%
#   change.donutuse.and.runinfo(28065.99,TRUE,"not enough gas to run") %>%

flatlist.Cyc <- flatlist.Cyc %>%
  change.donutuse.and.runinfo(29625.1, 29633.7,TRUE,"offset from the rest of population of dR_25, keep eye on")
  %>% #maybe throw out if later in clumped processing this sample varies in D47 space greatly
  change.donutuse.and.runinfo(30963.1, 30972,TRUE,"bulk isotopes offset from the rest of population of ETH1") %
  %>%
  change.donutuse.and.runinfo(31181.1, 31198.1,TRUE,"bulk isotopes offset from the rest of population of ETH2")
  %>%
  change.donutuse.and.runinfo(31392.1, 31397.1, TRUE, "sample too small") %>%
  change.donutuse.and.runinfo(31585.1, 31594.1, FALSE, "sample sat in trap 2 for ~60 mins bc of a FromPy read e
  rror between computers, keep an eye one") %>%
  #looking at the D47vsd47 plot, it appears to fall on top of all the other dR_25 and is not labelled at D4
  8excess... I'd keep for now
  change.donutuse.and.runinfo(31127.1, 31136.1, TRUE, "bulk isotopes offset from the rest of population of ETH
  1") %>%
  change.donutuse.and.runinfo(29378.1, 29383, TRUE, "bulk isotopes offset from rest of populations of ETH2") %
  %>%
  change.donutuse.and.runinfo(30341.1, 30362, TRUE, "unexplained long strain fo dR_25 and then 5 eSSB_25") %>%
  #dR_25 odd
  change.donutuse.and.runinfo(29255.1, 29264, TRUE, "dR_25 offset from rest of pop in bulk iso") %>%
  change.donutuse.and.runinfo(31809.1, 31818, FALSE, "ETH2 offset from rest of population, keep eye one") %>%
  #after looking at standard residuals for ETHs and identifying outliers that I am a fence about culling
  change.donutuse.and.runinfo(29369.1,29378, FALSE, "ETH1 outlier from rest of population") %>% #i think keep
  change.donutuse.and.runinfo(31809.1,31818, FALSE, "ETH2 outlier from rest of population") %>% #i think cull
  change.donutuse.and.runinfo(30895.1,30904, FALSE, "ETH3 high positive outlier from rest of population") %>% #
  batch 127. i think keep
  change.donutuse.and.runinfo(30250.1,30259, FALSE, "ETH3 high positive outlier from rest of population") %>% #
  batch 81. i think keep
  change.donutuse.and.runinfo(29351.1,29360, FALSE, "ETH3 negative outlier from rest of population") %>% #from
  20150520. batch 28. i think cull
  change.donutuse.and.runinfo(29652.1,29661, FALSE, "ETH3 negative outlierfrom rest of population") #from 2019
  0524. batch 50. i think cull

## note: eventually i need to look at the standard residuals and decide what time window of samples from May and
  June I want to keep and use for the dataframe for this date. Look at the standard residuals and decide when the c
  arbonate standards and the gases match the closest, and when the stdres's are lowest overall. that's the machine
  time window to use.
```

#clumped math with any outlier or for that matter the any bool

```
flatlist.Acq <- flatlist.Cyc %>%
  filter(Donutuse != TRUE) %>%
  clumpedCycToAcquisition()

flatlist.Acq.outlier<- flatlist.cyc.outlier(flatlist.Cyc, "Donutuse")

write.csv(flatlist.Acq, paste0(session, "_flatlist.Acq.csv"))
```

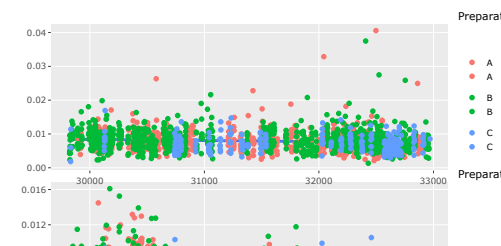
looking at bulk isotope stdev at the acquisition level

```
pd180 <- flatlist.Acq %>%
  filter(Donutuse != TRUE) %>%
  ggplot(aes(x=Analysis, y=d180.stdev)) +
  stat_smooth(method = "lm") +
  geom_point(aes(color=Preparation))

pd13C <- flatlist.Acq %>%
  filter(Donutuse != TRUE) %>%
  ggplot(aes(x=Analysis, y=d13C.stdev)) +
  stat_smooth(method = "lm") +
  geom_point(aes(color='Preparation'))

subplot(pd180,pd13C, nrow = 2)

## 'geom_smooth()' using formula 'y ~ x'
## 'geom_smooth()' using formula 'y ~ x'
```



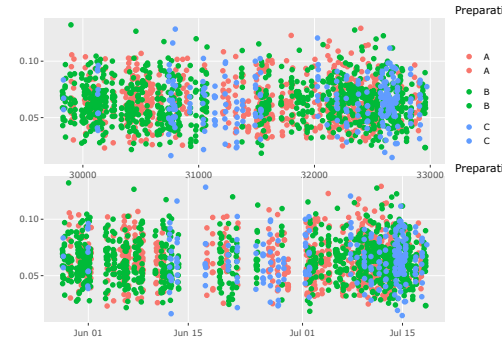
```

pD47 <- flatlist.Acq %>%
  filter(Donotuse != TRUE) %>%
  ggplot(aes(x=Analysis, y=D47.stdev, color='Preparation')) +
  geom_point()

pD47.date <- flatlist.Acq %>%
  filter(Donotuse != TRUE) %>%
  ggplot(aes(x=file_datetime, y=D47.stdev, color='Preparation')) +
  geom_point()

subplot(pD47,pD47.date,nrows = 2)

```



```

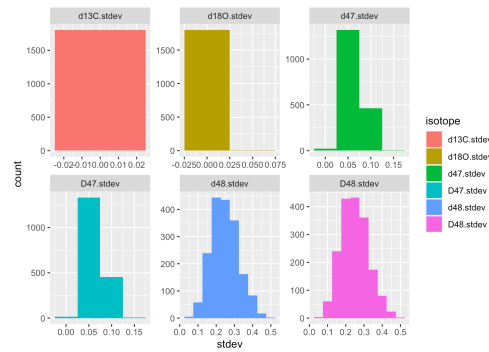
histograms <- flatlist.Acq %>%
  filter(Donotuse != TRUE) %>%
  gather(isotope, stdev, d13C.stdev, d18O.stdev, d47.stdev, d48.stdev, D47.stdev, D48.stdev)

acq.sd <- histograms %>%
  ggplot() +
  geom_histogram(aes(x=stdev, fill=isotope, binwidth = .05) +
  facet_wrap(isotope~., scales = "free")

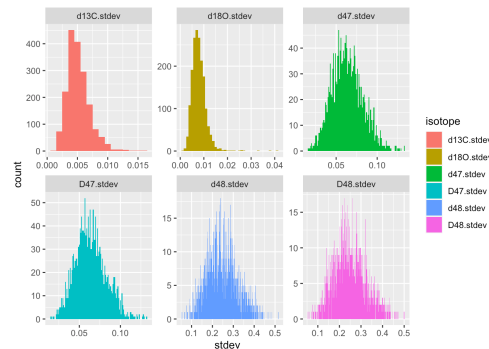
acq.sd2 <- histograms %>% filter(stdev < 2) %>%
  ggplot() +
  geom_histogram(aes(x=stdev, fill=isotope, binwidth = .001) +
  facet_wrap(isotope~., scales = "free")

acq.sd

```



acq.sd2



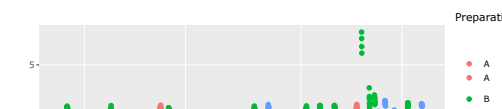
```

pD48 <- flatlist.Acq %>%
  filter(Donotuse != TRUE) %>%
  ggplot(aes(x=file_datetime, y=D48.full, color='Preparation', label = Identifier1)) +
  geom_point()

pD48 <- flatlist.Acq %>%
  filter(Donotuse != TRUE) %>%
  ggplot(aes(x=file_datetime, y=D48.stdev, color='Preparation', label = Identifier1)) +
  geom_point()

subplot(pD48,pD48,nrows = 2)

```



```
#last call for culling more samples, same syntax as above
```

Makes a new flatlist with each line as a sample for use in part 2 of the data processing procedures

```
standards.names <- c("TV04","Carrara.CIT", "ETH1","ETH2","ETH3")

flatlist.Sam <- flatlist.Acq %>%
  filter(Donotuse != TRUE) %>%
  group_by(batch.Aq) %>%
  summarise(
    Project = sub("\\$.*", "", sub("//$.*", "", `Identifier1`))[1],
    User = "",
    Date = file_datetime[1],
    Session = "NA",
    Sample.ID = sub("\\$.*", "", sub("/.$", "", `Identifier1`))[1],
    Type = if (Sample.ID %in% standards.names){
      "standard"
    }
    else if (sub("-", "*", "", Sample.ID) == "25")
    {
      "equilibrated gas"
    }
    else if (sub("-", "*", "", Sample.ID) == "1000")
    {
      "heated gas"
    }
    else{
      "sample"
    },
    Donotuse = Donotuse[1],
    runinfo = runinfo[1],
    spec.num = Analysis[1],
    mass.mas.numeric(`Identifier2` [1]),
    num.acqn(),
    Preparation = Preparation[1],
    Yield = Yield[1],
    Method = Method[1],
    d45.stdev= sd(d45),
    d45 = mean(d45),
    d46.stdev= sd(d46),
    d46 = mean(d46),
    d47.stdev= sd(d47),
    d47 = mean(d47),
    d48.stdev = sd(d48),
    d48 = mean(d48),
    d49.stdev = sd(d49),
    d49 = mean(d49),
    d47.stdev = sd(D47full),
    D47= mean(D47full),
    D48.stdev = sd(D48full),
    D48= mean(D48full),
    d13C.stdev= sd(d13C),
    d13C = mean(d13C),
    d180.stdev= sd(d180),
    d180.SHOW.gas = mean(d180),
    d180.VPDB.min = (((d180.SHOW.gas-30.86)/1.03086)+1000)/1.000211-1000, #acid fac and SHOW to
    PB= mean(PB),
    LeftPressure= mean(LeftPressure),
    RightPressure = mean(LeftPressure)
  )

write.csv(flatlist.Sam, paste0(session, "_flatlist.csv"))
```